NUMBER 1—JANUARY 1995

The corresponding states principle for radial distribution functions of homonuclear diatomic liquids By A. DE SANTIS, A. GREGORI and D. ROCCA	. 1
Nuclear spin relaxation in chloroform dissolved in a nematic phase: spectral densities at high frequencies	
By L. di Bari, L. Mäler and J. Kowalewski	31
Comment on 'Near critical phase behaviour of dilute mixtures' By A. A. CHIALVO and P. T. CUMMINGS	41
A Monte Carlo study of the condensed phases of biphenyl By A. Chakrabarti, S. Yashonath and C. N. R. Rao	49
N-Particle configurational integrals of model fluid-micropore systems By R. D. KAMINSKY	69
Analytical solution of the Ornstein-Zernike equation for mixtures By YIPING TANG and B. CY. LU	89
Non-additive forces in atomic clusters. The case of Ag,, By I. G. KAPLAN, R. SANTAMARIA and O. NOVARO	105
Identification of 1, 2 and 3 body Raman scattering by the field gradient induced dipole A tensor in	
methane	
By F. G. Baglin, E. J. Rose and S. Sweitzer Microscopic theoretical determination of the phase diagram of the hard core Yukawa fluid By C. Caccamo, G. Giunta and G. Malescio	115
The electric field gradient at the ⁹ Be nucleus in BeC	123
By A. C. Borin, F. R. Ornellas and L. T. Ueno	133
Water proton relaxation studies of pore microstructure in monodisperse glass bead beds By B. P. HILLS and J. E. M. SNAAR	141
Energy transfer between two mobile chromophores in a zero energy transfer configuration. Cross-correlation effects in the fluorescence anisotropy $r(t)$	
By I. I. FEDCHENIA and PO. WESTLUND	159
Capillary interface potential and interfacial fluctuations By A. Korociński and M. Napiórkowski	171
Calculating nuclear quadrupole coupling constants for van der Waals complexes By J. M. HUTSON	185
Fourier-transform infrared and jet-cooled diode-laser spectra of the 867 cm $^{-1}$ ν_{9} band of acetal-	165
dehyde By A. M. Andrews, M. Yu. Tretyakov, B. H. Pate, G. T. Fraser and I. Kleiner	201
Research Note	
Effective interactions in colloidal dispersions stabilized by free polymers	
By G. C. Barker, M. J. Grimson and M. Silbert	211
NUMBER 2—10 FEBRUARY 1995	
Monte Carlo simulation of liquid acetone with a polarizable molecular model By P. JEDLOVSZKY and G. PÁLINKÁS	217
Generalized collective modes for the Lennard-Jones fluid	
By I. M. MRYGLOD, I. P. OMELYAN and M. V. TOKARCHUK	235

Non-equilibrium molecular and Brownian dynamics simulations of shear thinning of inverse power	
fluids By D. M. Heyes and P. J. MITCHELL	261
High resolution FTIR spectrum of vinyl fluoride near 9 μ m: rovibrational analysis of the ν_{τ} band By P. Stoppa, S. Giorgianni, A. Gambi, A. de Lorenzi and S. Ghersetti	281
Rovibrational energy levels and transitions for H ₃ ⁺ computed from a new highly accurate potential energy surface	201
By R. JAQUET and R. RÖHSE Stability of fluids with more than two components. II. Demixing ternary mixtures of non-additive hard spheres	291
By D. Gazzillo	303
The solvation of cations in hydrogen-bonded molecular solvents: a neutron diffraction study on the structure of Ni ²⁺ solutions in ethylene glycol and in glycerol By S. E. OKAN, P. S. SALMON, D. C. CHAMPENEY and I. Petri	325
Molecular dynamics simulation of a needle-sphere binary mixture By K. Raghavan	345
New exact relations for the many-cavity distribution function of non-uniform hard-sphere systems By C. Rascón, G. Navascués and L. Mederos	373
Vapour-liquid equilibria of two-centre Lennard-Jones fluids from the NpT plus test particle method By C. Kriebel, A. Müller, J. Winkelmann and J. Fischer	381
Binary hard-sphere mixtures: a comparison between computer simulation and experiment By M. D. Eldridge, P. A. Madden, P. N. Pusey and P. Bartlett	395
The hard tetrahedron fluid: a model for the structure of water? By J. KOLAFA and I. NEZBEDA	421
Packing effects on the conformational equilibrium of alkanes By P. Padilla and C. Vega	435
NUMBER 3—20 FEBRUARY 1995	
Assessingly to Drive House	451
Appreciation to Brian Howard Theoretical studies of IR-UV sum frequency generation applied to adsorbed molecules By S. H. Lin, M. Hayashi, C. H. Lin, J. Yu, A. A. Villaeys and G. Y. C. Wu	451
Ab initio study of the structure of guanine-cytosine base pair conformers in gas phase and polar solvents	100
By J. Florián, J. Leszczyński and S. Scheiner	469
Quantum calculations of transport and relaxation properties for the helium-methane system	401
By F. A. GIANTURCO Magnetic angle selection in rhombic metal complexes and nitroxide radicals. EPR spectra as three-dimensional energy surfaces	481
By B. Kim, S. P. Greiner and R. W. Krelick	511
Charge separation/recombination reactions in non-polar fluids: a molecular description By D. V. Matyushov and R. Schmid	533
Quantum mechanical calculation of generalized collision cross-sections for the He-N ₂ interaction. Part II. Thermomagnetic effect By V. Vesovic, W. A. Wakeham, A. S. Dickinson, F. R. W. McCourt and M. Thachuk	553
A general pressure tensor calculation for molecular dynamics simulations	
By D. Brown and S. Neyertz	577
experiments	
By D. CANET, P. MUTZENHARDT and J. BRONDEAU	597
On the spin-orbit induced radiationless decay of the $b^3\Sigma^-$ state of BH	

A theoretical study of the rovibroaic spectra of CNO, NCO and CON By B. J. Persson, B. O. Roos and S. Carter	619
Nuclear spin-rotation interaction and non-Abelian gauge potential	627
By Yu. A. Serebrennikov and U. E. Steiner	027
NUMBER 4—MARCH 1995	
On the convergence rate of a cusp-corrected damped multipole expansion for the second-order H-H+ induction energy	622
By G. FIGARI, A. SICILIANO, C. COSTA and V. MAGNASCO	633
By V. Crupi, M. P. Jannelli, S. Magazu', G. Maisano, D. Majolino, P. Migliardo and D. Sirna	645
Numerical solution of the optimized random phase approximation By G. PASTORE, F. MATTHEWS, O. AKINLADE and Z. BADIRKHAN	653
Structure and ionization potentials of clusters containing heavy elements. Part 3: Mixed clusters of	033
alkali and group V elements By G. IGEL-MANN and H. STOLL	663
Structure and ionization potentials of clusters containing heavy elements. Part 4: Mixed clusters of alkali and group VI elements	679
By G. IGEL-MANN, R. SCHLUNK and H. STOLL. Quantum chemical predictions of the electron affinities of carbon-hydrogen clusters $C_{2n}H^*$, the CH binding energies and the gas phase acidities of polyacetylenes $C_{2n}H_2$ for $n=1-3$	
By J. NATTERER and W. KOCH	691
By J. Cioslowski and B. B. Stefanov	707
A coupled-cluster study of the molecular structure, vibrational spectrum and relative energies of the XCN and XNC (X = F, Cl) isomers By T. J. Lee and S. C. RACINE	717
Molecular dynamics study of the plastic-crystalline phase transition of tetraphosphorus triselenide By A. Sergi, M. Ferrario, S. R. Elliott and I. R. McDonald	727
A fast method of solving the hypernetted-chain equation for molecular Lennard-Jones fluids By J. A. Anta, E. Lomba, C. Martín, M. Lombardero and F. Lado	743
Can the 'van der Waals loop' vanish? II. Effect of domain size By R. Yamamoto, O. Kitao and K. Nakanishi	757
A far infrared study of water diluted in hydrophobic solvents By T. Tassaing, Y. Danten, M. Besnard, E. Zoidis, J. Yarwood, Y. Guissani and	
B. GUILLOT Polarizabilities of anions in anisotropic environments. The fluoride ion in the perovskite lattices	769
NaMgF ₃ , KMgF ₃ and KCaF ₃ By P. W. Fowler, F. Ding and R. W. Munn	787
The structure of a hard sphere fluid restricted by permeable walls By P. Marsh, G. Rickayzen and M. Calleja	799
Erratum	
Formulae for the first and second derivatives of anisotropic potentials with respect to geometrical parameters By P. L. A. POPELIER and A. J. STONE	811
NUMBER 5—10 APRIL 1995	
One-centre multipole calculation of second-order perturbation energies for H ₂ ⁺ By V. Magnasco, G. Figari, A. Siciliano and M. Rui	813

Liquid-liquid phase transitions in pores	
By W. T. Góźdź, K. E. Gubbins and A. Z. Panagiotopoulos	825
Analytical solutions for spin 7/2 line intensities in solid state NMR By S. Z. AGEEV and B. C. SANCTUARY	835
Fourier path integral simulations of para-H ₂ and ortho-D ₂ clusters By C. CHAKRAVARTY	845
Rovibrational Hamiltonian for molecular complexes	045
By J. Makarewicz and A. Bauder	853
A systematic model potential for Li ⁺ -H ₂ O By R. J. Wheatley and J. M. Hutson	879
The non-additive exchange energies of H ₃ and He ₃ By R. J. WHEATLEY	899
External magnetic field acceleration of radiationless processes in the $\widetilde{\mathbf{A}}$ state of gaseous oxalyl fluoride	
By V. I. Makarov, Haruo Abe and Hisaharu Hayashi	911
Reversion of magnetic field effects under large magnetic fields observed in the photochemical hydrogen abstraction reactions of fluorinated acetophenone and benzophenone in micellar solutions By Masatoshi Igarashi, Qing-Xiang Meng, Yoshio Sakaguchi and Hisaharu	
HAYASHI	943
Quasiclassical trajectory study of the Li + Cs ₂ reaction By V. M. F. Morais and A. J. C. Varandas	957
Quantum calculations of multistructure cross-sections for the Ca(4s5p, ${}^{3}P_{2}\leftarrow {}^{1}P_{1})$ + He collisional	
By E. Paul-Kwiek and T. Orlikowski	971
Interference of heavy-atom with magnetic spin effects in spin-correlated micellar radical pairs By Jie Quang Wu, D. Baumann and U. E. Steiner	981
RF-driven and proton-driven NMR polarization transfer for investigating local order. An application to solid polymers By P. ROBYR, M. TOMASELLI, J. STRAKA, C. GROB-PISANO, U. W. SUTER, B. H. MEIER	
and R. R. Ernst	995
High pressure NMR study of methyl group tunnelling in dimethyl sulphide By P. J. McDonald and M. Pinter-Krainer	1021
Theory of an excess electron in fluid helium. The effect of non-pairwise additivity of the solvent-induced interactions	
By Jun Wang and A. D. J. Haymet	1033
Research Note	
Influence of surface and torsion potentials on the melting properties of a hexane monolayer on a graphite substrate. A molecular dynamics simulation study	
By G. H. Peters and E. Velasco	1039
NUMBER 6—20 APRIL 1995	
Free energy and entropy production in planar Couette flow far from equilibrium By M. Peric and G. P. Morriss	1049
An associative version of the Henderson-Abraham-Barker equation By M. F. HOLOVKO and E. V. VAKARIN	1057
Translational absorption band in low density mixtures of noble gases: the He-Xe case By P. Dore, L. Finzi, A. Nucara, P. Postorino and M. Rovere	1065
Implicit discretization schemes for Langevin dynamics	1003
By G. ZHANG and T. SCHLICK	1077
Model of adsorption at a fluid-fluid interface By S. J. Bibb, J. S. Rowlinson and C. Xiao	1099

Chromium dihydride (CrH ₂): theoretical evidence for a bent ⁵ B ₂ ground state By B. J. DeLeeuw, Y. Yamaguchi and H. F. Schaefer III	1109
Resolution of the sign problem in quantum Monte Carlo simulations of annulenes By J. SCHÜTT, J. SCHULTE, M. C. BÖHM and Z. G. Soos	1127
Water adsorption in microporous graphitic carbons By D. E. Ulberg and K. E. Gubbins	1139
Counterpropagating molecular beam scattering of NH ₃ + nH ₂ By H. MEYER	1155
An analysis of the magnetizability tensor at CHF level By M. J. PACKER and B. T. PICKUP	1179
A new twist to molecular chirality: intrinsic chirality indices By M. A. OSIPOV, B. T. PICKUP and D. A. DUNMUR	1193
A molecular dynamics interpretation of the inelastic neutron spectra in the plastic phase of hexachloroethane By A. MuÑoz and A. CRIADO	1207
Local structure in anisotropic systems determined by molecular dynamics simulation. Application to a nematic liquid crystal By A. V. KOMOLKIN and A. MALINIAK	1227
Vibrational averaging of electrical properties Development of a routine theoretical method for polyatomic molecules By A. J. RUSSELL and M. A. SPACKMAN	1239
Hydrogen bond dynamics in tetrafluoroterephthalic acid studied by NMR and INS By A. J. Horsewill, A. Ikram and I. B. I. Tomsah	1257
Research Note	
On the use of a non-additive reference system in a reference hypernetted chain calculation of the structure of a binary liquid	
By J. A. Anta and G. Kahl	1273